

# ADVANCED REACTOR, FUEL CYCLE, AND ENERGY PRODUCTS WORKSHOP FOR UNIVERSITIES

---

## Advanced Fuel Development

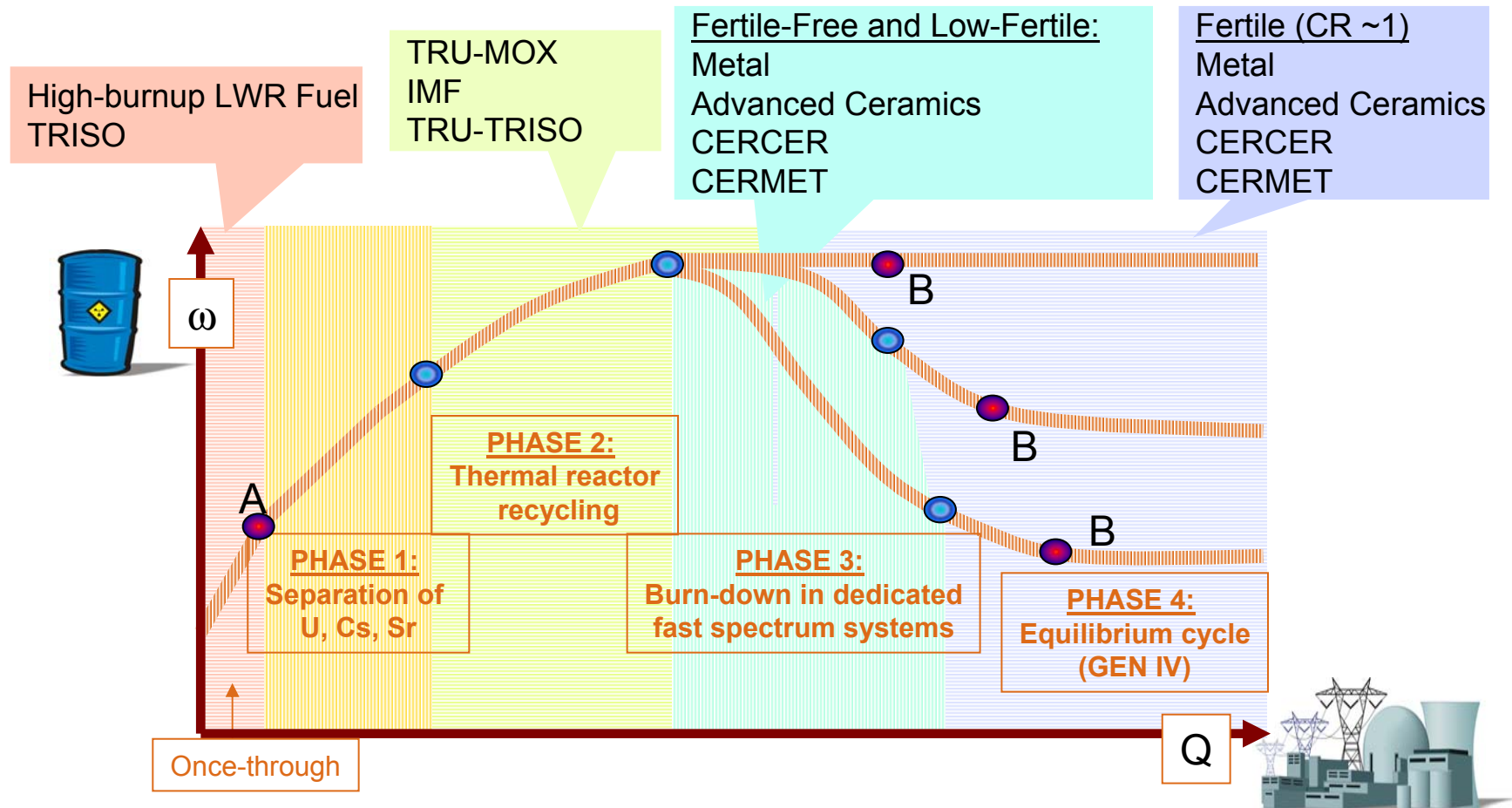
**Kemal O. Pasamehmetoglu**

**National Technical Director ([kop@lanl.gov](mailto:kop@lanl.gov))**

*Workshop for Universities  
Hilton Hotel, Gaithersburg, MD  
March 4-5, 2004*

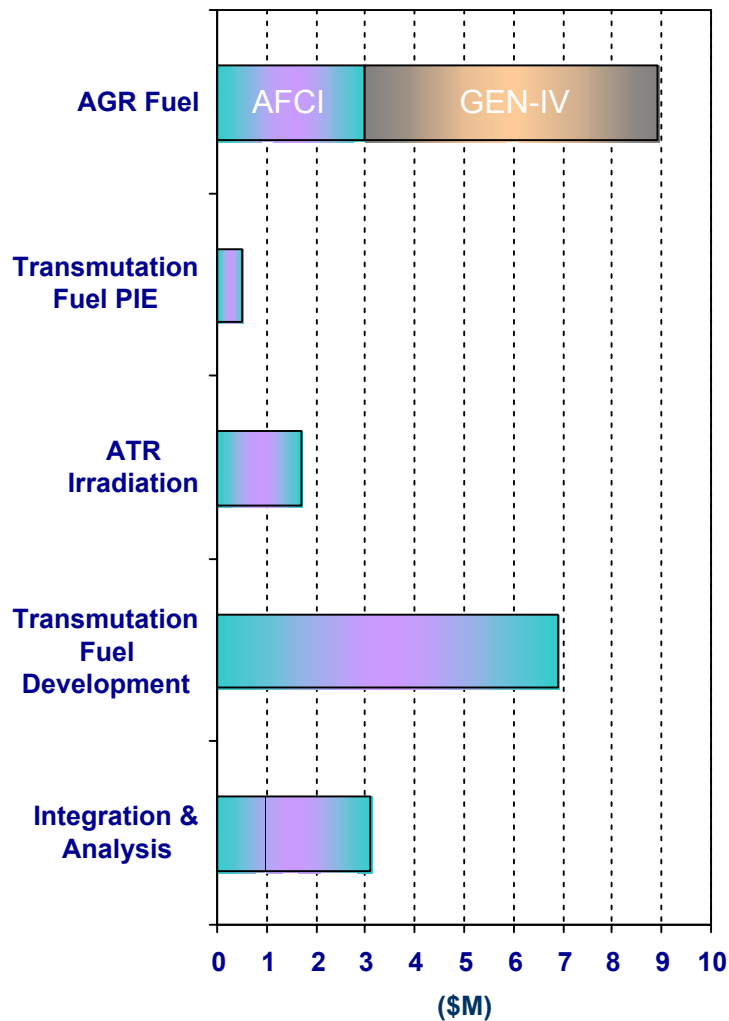


*The fuel development program covers fuels and cladding research for multiple phases of the fuel cycle evolution . The scope keeps growing...*



$\omega = F(\text{volume, radiological risk, short-term heat load, long-term heat load, plutonium mine})$

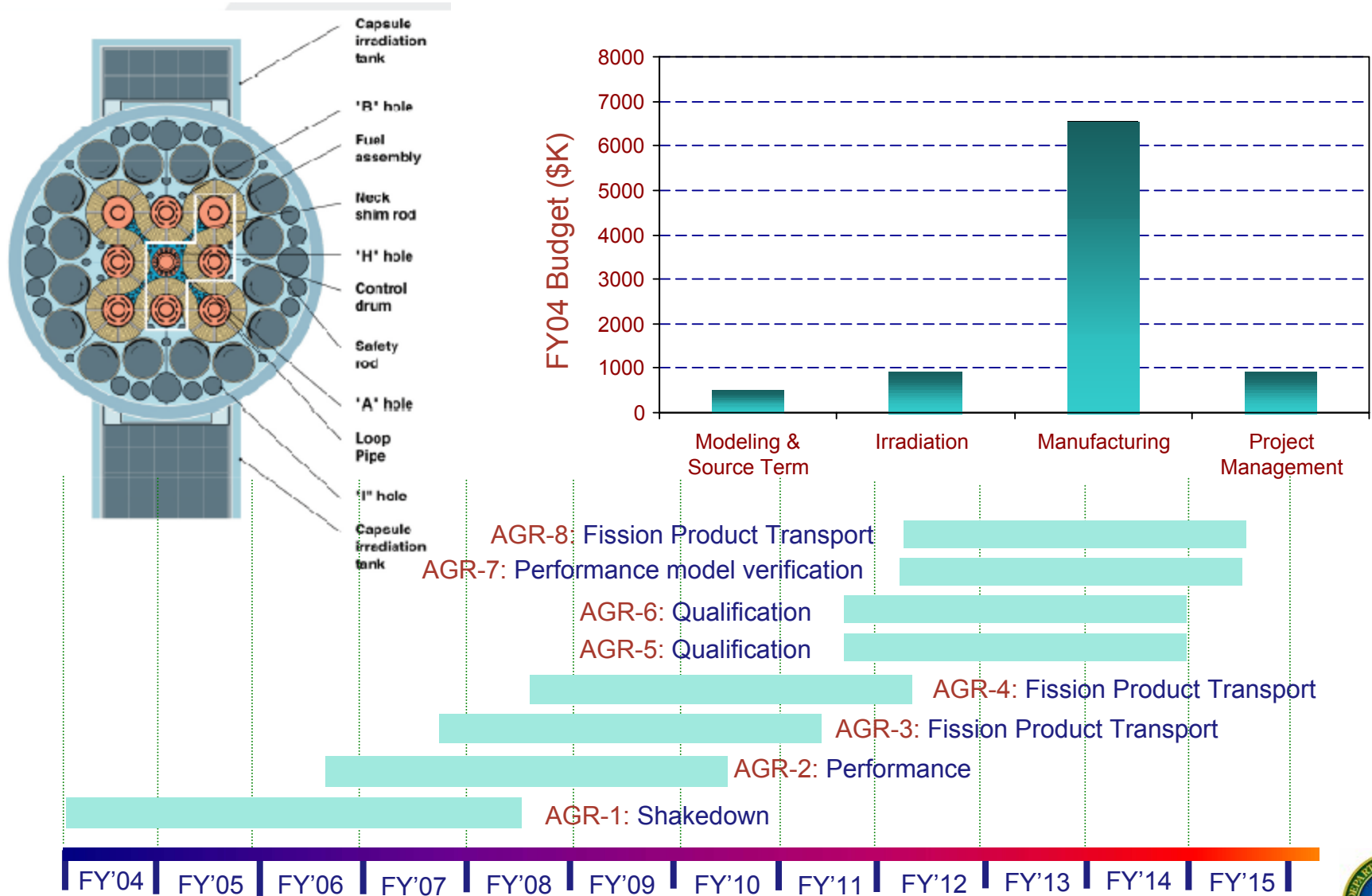
*In FY04, the total budget of fuel development activities is \$21 M.*



- AGR Fuel
  - UCO TRISO fuel development with emphasis on fuel manufacturing for AGR-1 test in ATR
- Transmutation fuel PIE
  - GE-2000 cask interface design for transferring ATR samples to HFEF.
- ATR Irradiation
  - LWR-1 Tests (mixed oxide with Np)
  - AFC-1 Irradiations (low-fertile and non-fertile metal and nitride fuels)
  - GFR-1 Irradiation (dispersion fuel matrix materials for gas fast reactor)
- Transmutation Fuel Development
  - Process development, fabrication and characterization of
    - Mixed oxide fuels
    - Nitride fuels
    - Metal fuels
    - Dispersion fuels
- Integration and Analyses
  - Project management
  - Analyses (e.g. IMF implementation)
  - International collaborations (FUTURIX)
  - University support (R&D contracts, student and professor support)



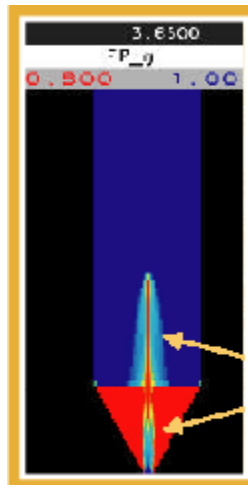
# The FY'04 emphasis of TRISO fuel development is the particle fuel fabrication for the shake-down test in ATR



### Scope and Objectives

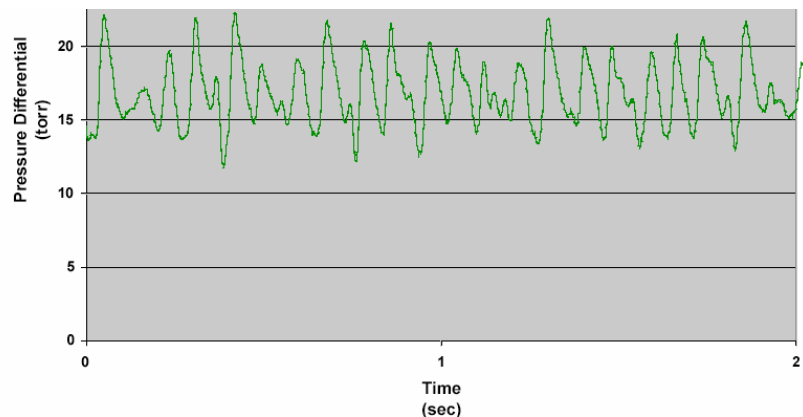
- Develop coating technology with the objective to meet the German standards.
- Test the coated particles in ATR to assess the irradiation performance.
- Transfer coating technology to BWXT for commercial scale fabrication.
- Develop and validate the MFIX code used for modeling the coating process (Chemical Vapor Deposition in a fluidized bed).

PI: Dave Williams  
e-mail: [williamsdf2@ornl.gov](mailto:williamsdf2@ornl.gov)



### Accomplishments

- Considerable amount of coating testing is being done at ORNL using primarily surrogate materials using a small coater (2-in coater).
- MFIX code is being run and compared to data obtained using the small coaters. Experimental and analytical work is being carried out in collaboration with University of Tennessee.

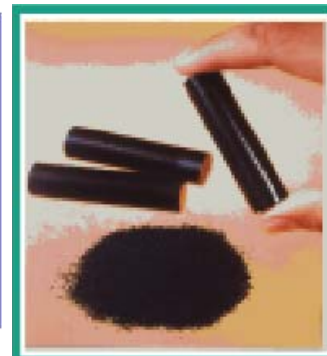




### Scope

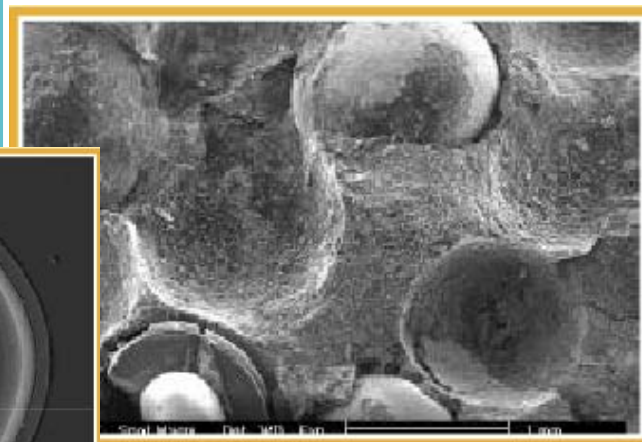
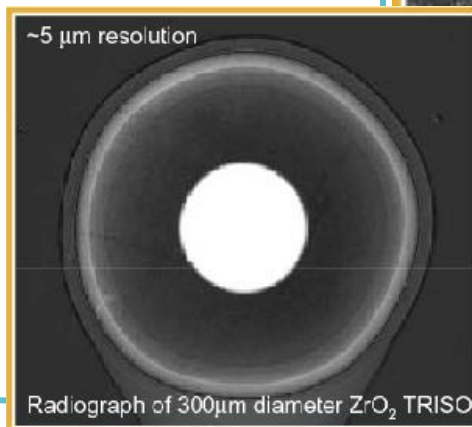
- Develop compacts for TRISO fuel that meet the German irradiation performance standards.
- Develop the over-coating technology that reduces the pressure on the particles during the compacting process.
- Characterize the archived German particles
- Develop advanced characterization techniques
- Transfer compacting and characterization technologies for industrial use.

*PI: Dave Williams  
e-mail: [williamsdf2@ornl.gov](mailto:williamsdf2@ornl.gov)*



### Accomplishments

- Overcoating technology is being developed to minimize the potential particle damage during compacting.
- Characterization of German particles is ongoing.
- Advanced characterization technologies:
  - Non-destructive testing
  - Automated characterization



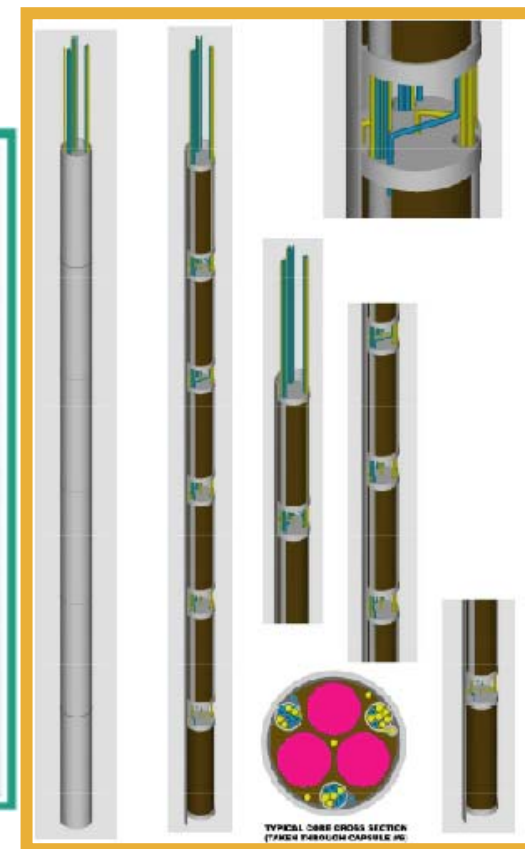
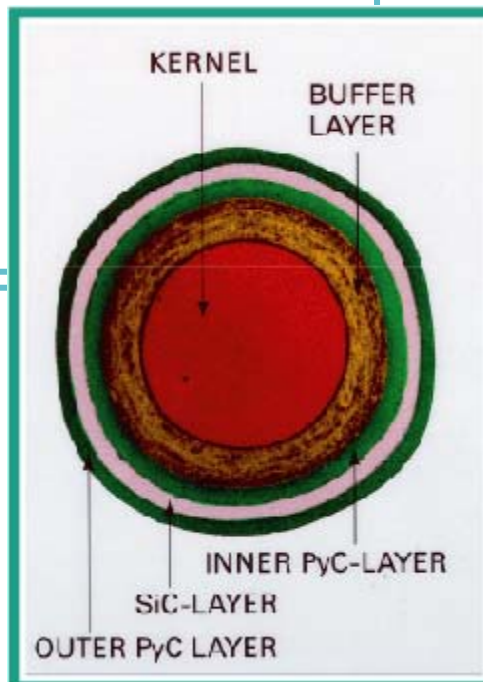
### Scope

- Fabrication, testing and qualification of UCO fuel particles for use in VHTR.
- Series of tests in AGR under NQA-1 in ATR 2005 - 2012 leading to fuel qualification.

*PI: Dave Petti  
e-mail: [pti@inel.gov](mailto:pti@inel.gov)*

### Accomplishments

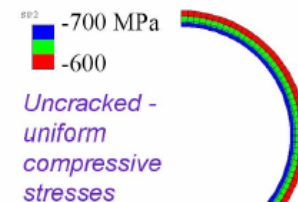
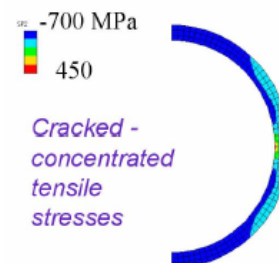
- Fabricated LEO2, NUOC kernels
- Kernels are being shipped to ORNL for coating and compacting.
- Conceptual design of AGR-1 is completed.



### Scope

1. Properties of fuel coating layers under normal operation (NERI) & properties of fuel coating layers under accident conditions (French I- NERI)
2. Code Benchmarking
  - In FY 2004, the actual PARFUME calculations for the eight benchmarking cases will be performed.
3. Develop improved accident code
  - PARFUME code modifications to address accident conditions and performance of calculations under both heating test conditions and conduction cool down conditions.
4. Document status of benchmark calculations and code improvement work (Sept. 30, 04)

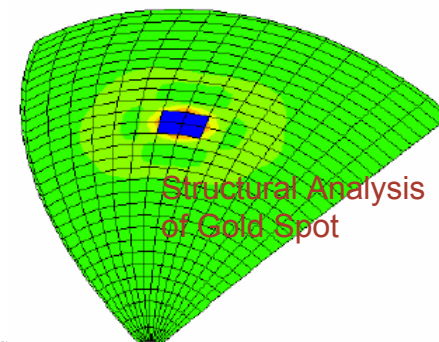
*PI: Dave Petti  
e-mail: [pti@inel.gov](mailto:pti@inel.gov)*



### Accomplishments

- PARFUME is being used to analyze a number of various scenarios for TRISO particles
  - Cracked coating
  - Delamination and gold spot
- TMAP model (1D diffusion through the particle fuel) is being developed and benchmarked to be used for fission product transport and source term calculations

Structural Analysis of Asphericity



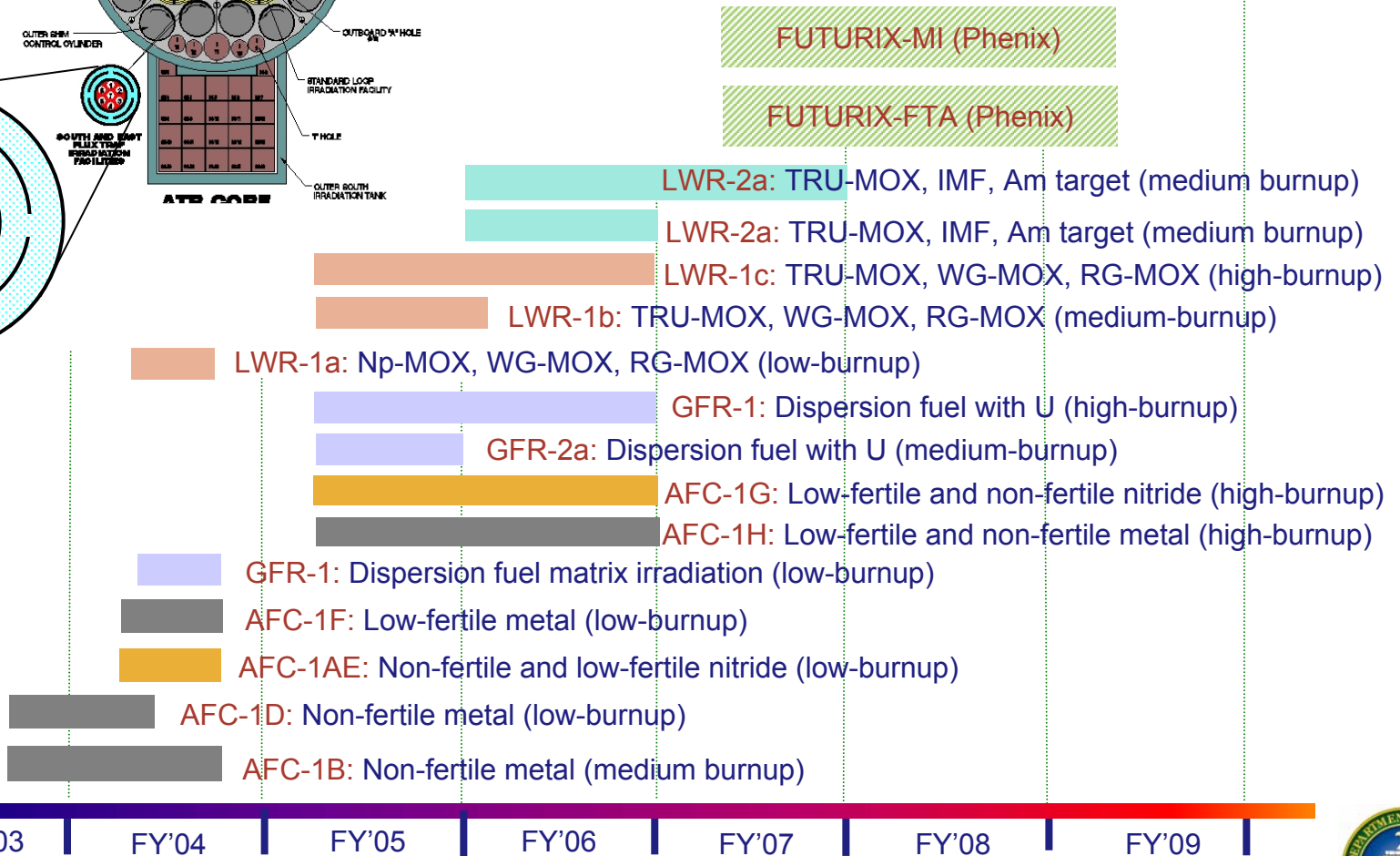
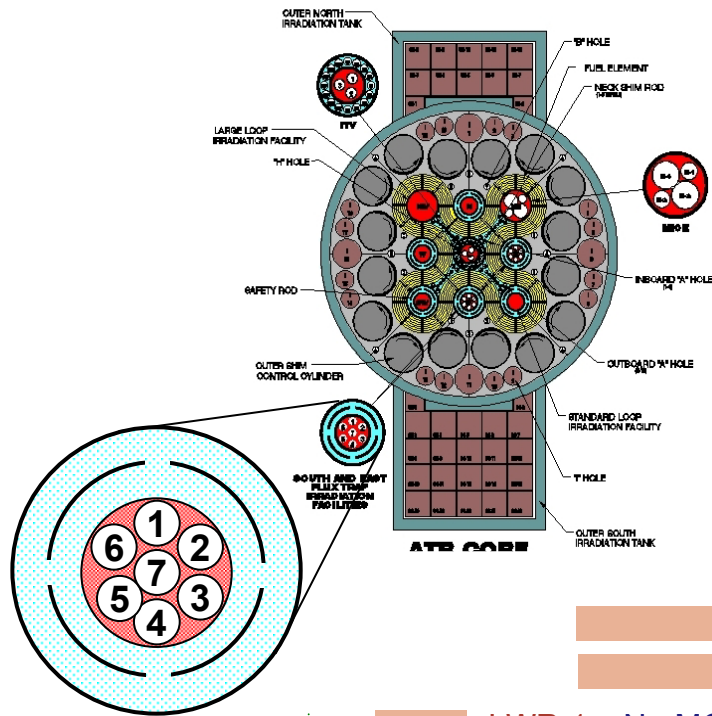


*Some specific University research areas of interest for the TRISO fuel development are*

- Evaluation and Development of Thermocouples for High Temperature Nuclear Environments in the Advanced Test Reactor, Idaho National Lab.
- Optimization of the gamma-ray detector types for Advanced Test Reactor (ATR) fission product monitoring system
- Methods to evaluate and limit fission product plating in ATR fission product monitoring system tubing
- Thermochemical Analysis of Multi-Composition Kernels for Coated Particle Fuel
- High Temperature Gettering of Cesium, Silver, Iodine, and Tellurium in Advanced Gas Cooled Reactors
- Evaluation of natural graphite properties after adsorption of fission products
- Compacting development evaluation and innovative methods
- Detailed reaction kinetics for CVD process and incorporation into MFIIX
- Experimental and numerical investigation of 6-inch coater hydrodynamics



*ATR irradiation and PIE for transmutation involve mixed-oxide, IMF, americium targets, nitride, metal and dispersion fuels.*



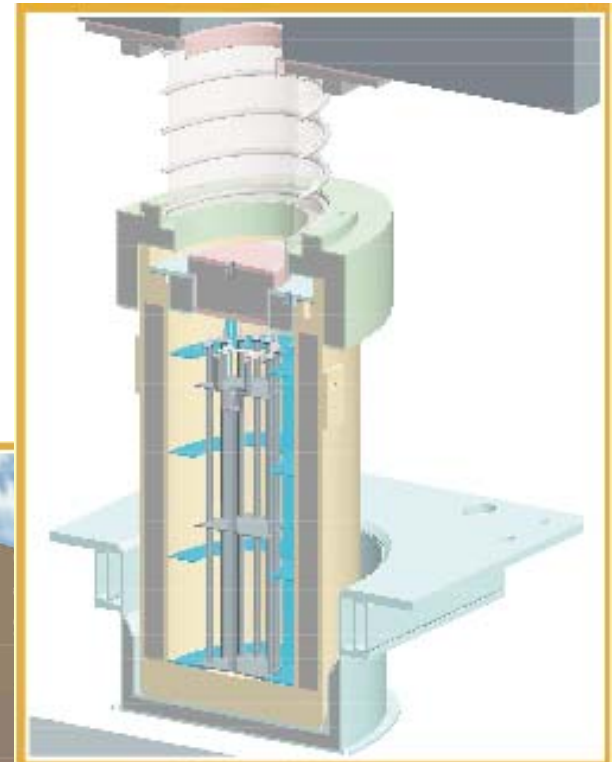
### Scope

- Preparation of the GE-2000 interface at HFEF
- Subsequent PIE of samples from the following tests
  - AFC-1
  - LWR-1 & 2,
  - GFR-1, 2 & 3
- PIE on cadmium baskets
- FUTURIX FTA and MI PIE will be performed at HFEF (ANL) and CMR (LANL) hot cells

*PI: Bruce Hilton  
e-mail: [bruce.hilton@anl.gov](mailto:bruce.hilton@anl.gov)*

### Accomplishments

The HFEF will be ready to start the PIE on the samples from irradiations experiments by late summer'04



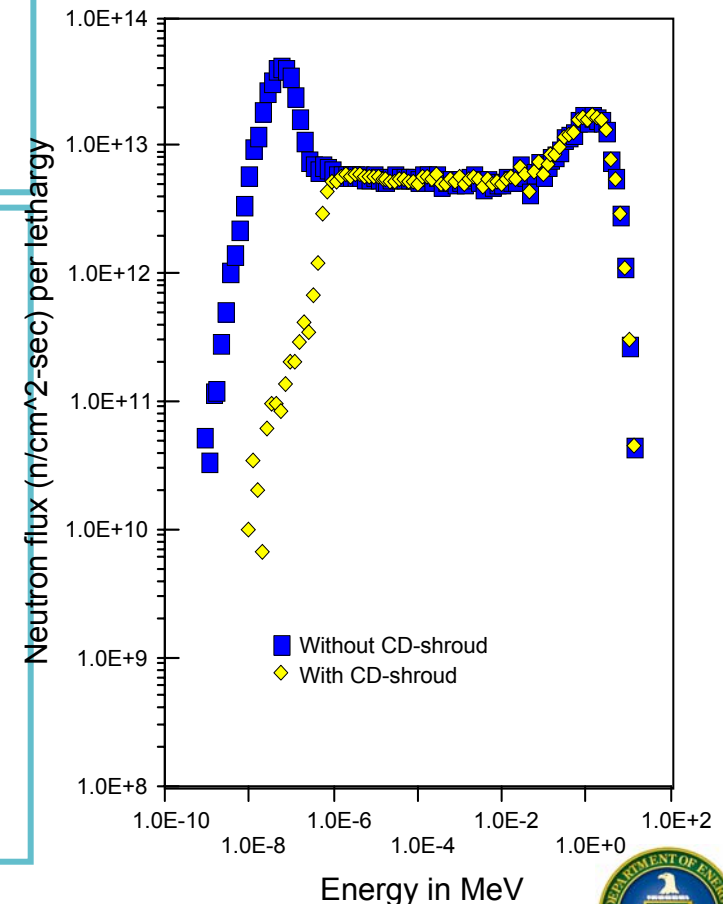
### Scope

- Design, analyze and conduct irradiation tests for fast and thermal spectrum transmutation fuels in ATR.
- Prepare and get approval on necessary safety documentation

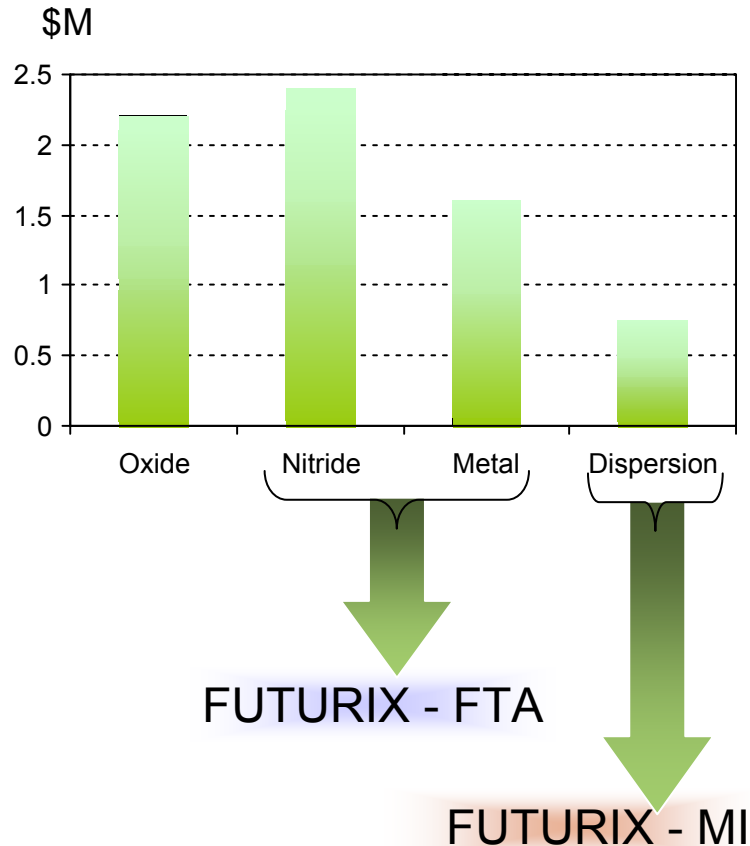
### Accomplishments

- AFC-1, LWR-1, GFR-1 tests are ongoing
  - AFC-1: Non-fertile, and low-fertile metal and nitride fuels containing U, Pu, Np, Am (low and intermediate burnup)
  - LWR-1: Np-MOX fuel, low burnup
  - GFR-1: Matrix materials for GFR-1
- Preparing for the next series after core-change-out
  - AFC-1 G & H: high burnup metal and nitride fuels
  - AFC-1B: high burnup for TRU-MOX
  - LWR-2: TRU-MOX, TRU-IMF, Am targets

PI: Richard Ambrosek  
e-mail: [rga@inel.gov](mailto:rga@inel.gov)



## *Transmutation Fuel Development is a major focus of the AFCI program*



- Oxide Fuels
  - TRU containing mixed oxide fuel process development fabrication and characterization
  - Modeling
- Nitride Fuels
  - TRU containing fertile-free or low-fertile nitride fuel process development fabrication and characterization
  - Modeling
- Metal Fuels
  - TRU containing fertile-free or low-fertile metal fuel process development fabrication and characterization
  - Modeling
- Dispersion Fuels
  - GFR fuel matrix materials development
  - Aluminide matrix assessment





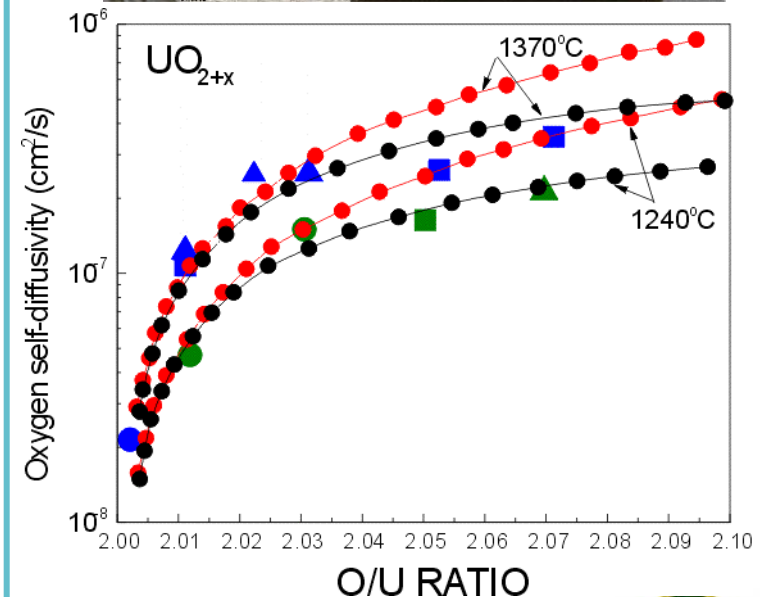
### Scope

- Fabrication process development and characterization of TRU bearing oxide fuels for fast spectrum transmutation
  - Low-fertile and non-fertile
- Modeling of fabrication processes and irradiation performance of TRU-bearing metal fuels

### Accomplishments

- Initial set of Np-Pu-U mixed oxide fuels were fabricated and characterized.
- They are being irradiated in ATR for a side-by-side comparison with weapons-grade and reactor-grade MOX fuels.
- Process optimization tests are ongoing
- High-burnup fuels are being fabricated
  - Including the investigation of incorporating Am into the fuel.
- Oxygen diffusion model development and analyses started.
- Synthesis model to support the feed preparation started.
- Heat transfer (TRUCHAS) model for the fuel pins started

*PI: Stuart Maloy  
e-mail: maloy@lanl.gov*



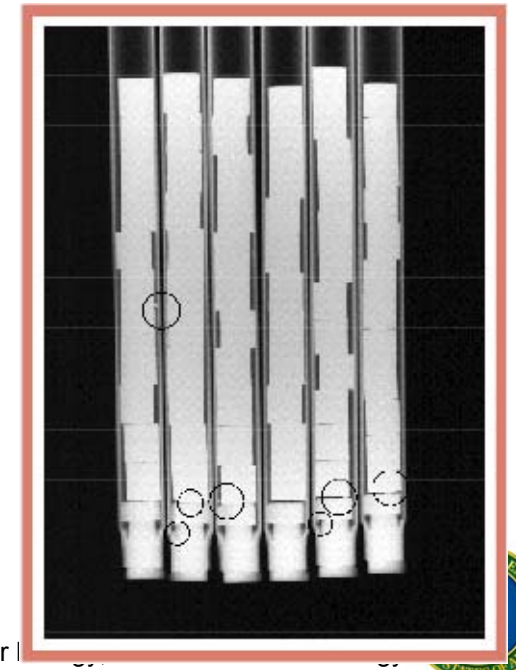
### Scope

- Fabrication process development and characterization of TRU bearing nitride fuels for fast spectrum transmutation
  - Low-fertile and non-fertile
- Modeling of fabrication processes and irradiation performance of TRU-bearing nitride fuels

*PI: Stuart Maloy  
e-mail: [maloy@lanl.gov](mailto:maloy@lanl.gov)*

### Accomplishments

- A series fertile-free and low-fertile (Pu-Np-Am-Zr) nitride pellets have been fabricated and characterized
- They are being irradiated at ATR to low-burnup
- Fabrication of high-burnup fuel pellets continue
- Process optimization tests are ongoing
- Surrogate (ZrN) and real nitride pellets are being fabricated for thermal diffusivity measurements and sodium bonding tests to be conducted at ANL.
- Nitride phase diagram modeling activities continue.
- The ion-beam irradiated samples of ZrN are being analyzed for helium-release and radiation damage.
- Collaboration with ASU continues to assess microstructural evolution and mechanical properties of nitrides



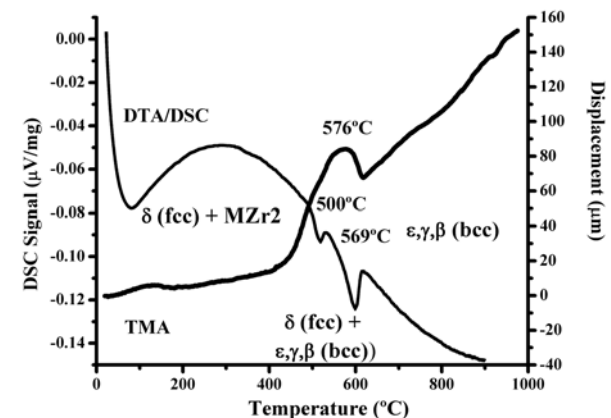
### Scope

- Fabrication process development and characterization of TRU bearing metal fuels for fast spectrum transmutation
  - Low-fertile and non-fertile
- Modeling of fabrication processes and irradiation performance of TRU-bearing metal fuels

### Accomplishments

- A series of low-fertile and non-fertile metal fuels have been fabricated, characterized and are being irradiated in ATR
- Microstructure/phase equilibria, thermal analyses and thermal conductivity of AFC-1 and FUTURIX fuels continue, with early emphasis on thermal analyses.
- Improved sodium bonding process development tests are starting soon.

*PI: Steve Hayes  
e-mail: [steven.hayes@anl.gov](mailto:steven.hayes@anl.gov)*



Before

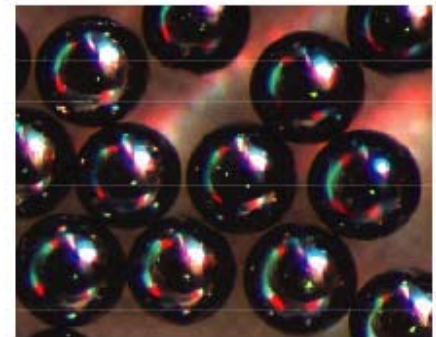


After

### Scope

- Define dispersion fuel concepts for fast reactor applications
  - Emphasis on GFR
- Develop and test matrix materials
- Fabrication process development and characterization of TRU bearing dispersion fuels for fast reactors and fast spectrum transmutation
  - Low-fertile and non-fertile
- Modeling of fabrication processes and irradiation performance of TRU-bearing dispersion fuels

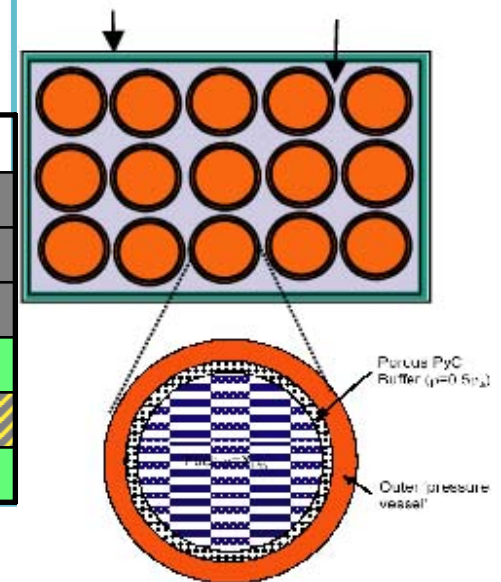
*PI: Mitch Meyer  
e-mail: mitchell.meyer@anl.gov*



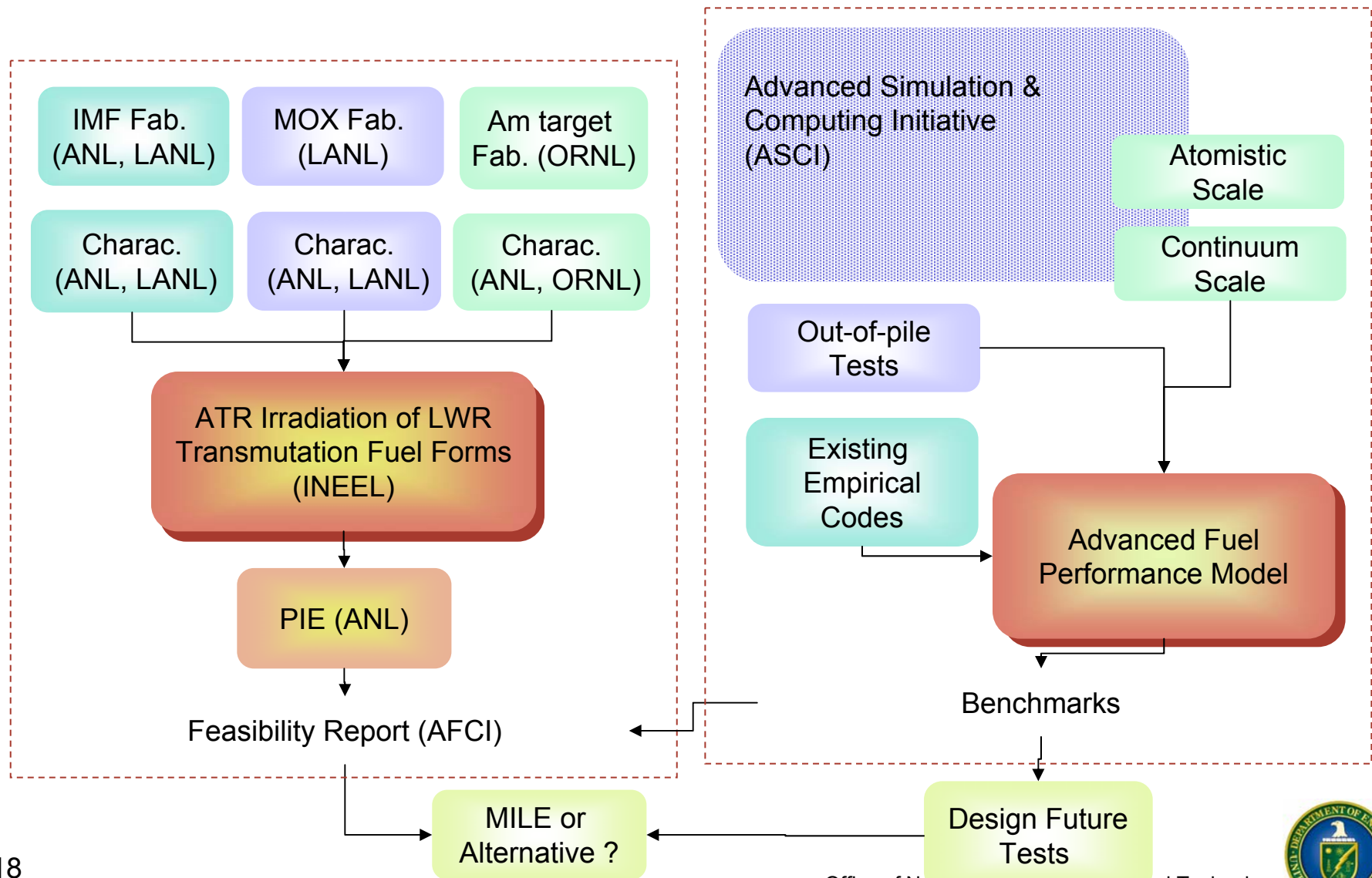
### Accomplishments

- Initial screening of potential matrix materials completed
- A materials irradiation test in ATR prepared and irradiation started
- Negotiations continue for FUTURIX-MI collaboration with CEA.
- Modeling efforts started
- Particle fabrication methods are being assessed

Oxides	Carbides	Nitrides
Al <sub>2</sub> O <sub>3</sub>	SiC	AlN
CeO <sub>2</sub>	TiC	CeN
MgAl <sub>2</sub> O <sub>4</sub>	VC	Si <sub>3</sub> N <sub>4</sub>
MgO	YC <sub>2</sub>	TiN
Y <sub>2</sub> O <sub>3</sub>	ZrC	YN
ZrO <sub>2</sub>		ZrN



*Two major US-lead initiatives are being planned to focus relevant National and International research*





# Models and Simulations, Short-Term

PI: Marius Stan  
e-mail: [mastan@lanl.gov](mailto:mastan@lanl.gov)

Phase diagrams show conflicting info (ex. UN stoichiometry)



U-N and Pu-N phase diagrams  
via thermo-chemistry

Mechanism and kinetics of species diffusion in ceramics unclear



Model of oxygen  
diffusion of in  $\text{PuO}_{2-x}$  and  
 $\text{UO}_{2\pm x}$

Models of mechanical properties  
must be predictive



Constitutive model of ZrN

Optimization of the carbo-thermal  
reduction process is needed



Thermochemical model  
of oxide feed preparation

Thermo-mechanical  
properties in fuel codes



Simulation of heat transfer in  
oxide fuels using FRAPCON  
and TRUCHAS



# Models and Simulations, Long-Term

PI: Marius Stan  
e-mail: [mastan@lanl.gov](mailto:mastan@lanl.gov)

Important phase diagrams  
are not known



Am-N phase diagram via  
atomistic modeling



Np-N phase diagram via  
atomistic modeling

Thermo-mechanical properties of  
new nitride compounds needed



Electronic Structure  
calculations of temperature  
effects in nitrides

Multi-component phase  
diagrams needed (U-Np-Pu-Zr)



Assessment of the  
Pu-Zr phase diagram



Assessment of the  
Np-Zr phase diagram



Assessment of the  
Pu-Np-Zr phase diagram

Defects formation and species  
mobility unclear

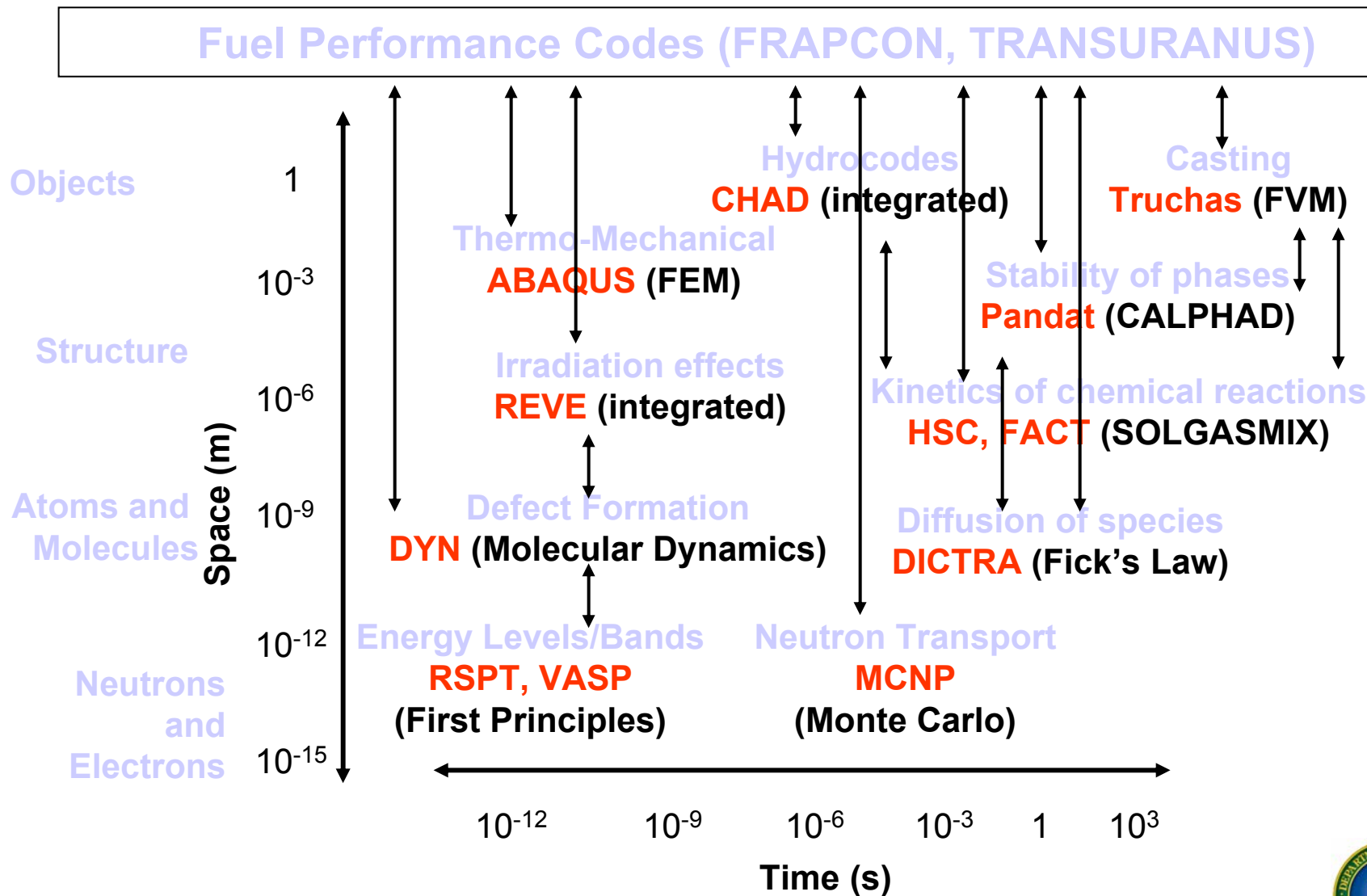


Add charge transfer to atomic  
potentials and do accelerated  
molecular dynamics simulations



# Scales/Codes/Methods

PI: Marius Stan  
e-mail: [mastan@lanl.gov](mailto:mastan@lanl.gov)



# *Workshops on Materials Modeling and Simulations For Nuclear Fuels*

*organized by the AFCI/LANL Modeling Team*

MMSNF-1, June 9-10, 2003, Santa Fe, NM

[www.lanl.gov/orgs/mst/nuclearfuels/](http://www.lanl.gov/orgs/mst/nuclearfuels/)

MMSNF-2, November 20-21, 2004, New Orleans, LA

[www.lanl.gov/orgs/mst/mmsnf/](http://www.lanl.gov/orgs/mst/mmsnf/)

**New ! MMSNF-3, June 17-18, 2004, Pittsburgh, PA**

**Following the ANS Summer Meeting**

*For information, contact Marius Stan at [mastan@lanl.gov](mailto:mastan@lanl.gov)*



Non-Fertile Fuels

(48)Pu-12Am-40Zr

(Pu<sub>0.50</sub>, Am<sub>0.50</sub>)N + 36-wt%ZrN

(Pu<sub>0.20</sub>, Am<sub>0.80</sub>)O<sub>2</sub> + 65-vol%MgO

(Pu<sub>0.50</sub>, Am<sub>0.50</sub>)O<sub>2</sub> + 70-vol%MgO

(Pu<sub>0.23</sub>, Am<sub>0.25</sub>, Zr<sub>0.52</sub>)O<sub>2</sub> + 60-vol%Mo<sup>92</sup> He

(Pu<sub>0.50</sub>, Am<sub>0.50</sub>)O<sub>2</sub> + 60-vol% Mo<sup>92</sup>

Low-Fertile Fuels

(35)U-29Pu-4Am-2Np-30Zr

(U<sub>0.50</sub>, Pu<sub>0.25</sub>, Am<sub>0.15</sub>, Np<sub>0.10</sub>)N

Bond

Na

Na

He

He

ITU

He

Na

Na

Fabricator

ANL

LANL

CEA

CEA

ITU

ITU

ANL

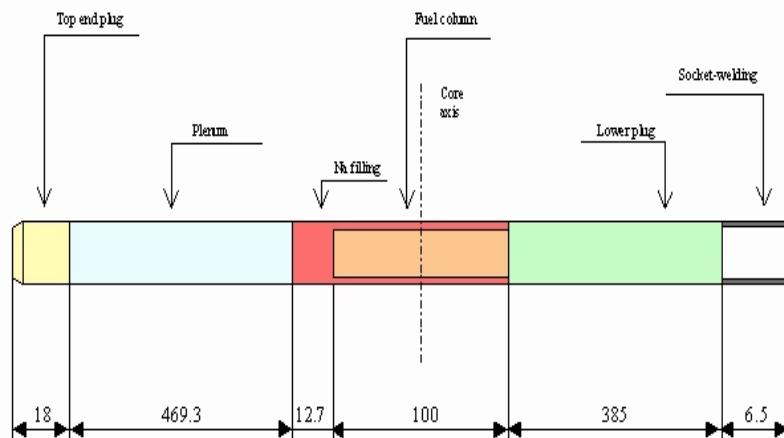
LANL

PI: Steve Hayes

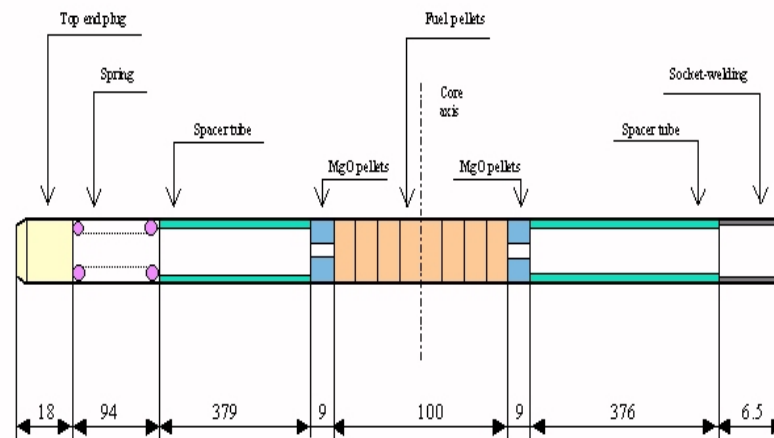
e-mail: [steven.hayes@anl.gov](mailto:steven.hayes@anl.gov)

19-pin experimental subassembly to be used

- 8 experimental pins
  - 11 standard Phénix driver pins or dummies
- Irradiation in Phénix ring 3 or 4
- Satisfies LHGR limit of 350 W/cm



Na-bonded fuels



He-bonded fuels



**EFFECT OF IRRADIATION ON PHYSICAL AND  
CHEMICAL PROPERTIES**

- DENSITY (SWELLING)
- MICROSTRUCTURE
- COMPOSITION - CRYSTALLOGRAPHIC PHASES
- ACTIVATION
- THERMAL PROPERTIES : Thermal Conductivity, Thermal Diffusivity, Heat Capacity, Linear Expansion
- MECHANICAL PROPERTIES : Young Modulus, Poisson ration, Hardness, Strength
- ELECTRICAL RESISTIVITY

PI: Mitch Meyer  
e-mail: [mitchell.meyer@anl.gov](mailto:mitchell.meyer@anl.gov)

**INERT MATERIALS**

$\alpha$ -SiC : 2 types (mono and polycrystal)

$\beta$ -SiC: 2 types ( mono and polycrystal)

ZrC : 2 types (micro and sub-micro.)

TiC

TiN

ZrN

Mo (Alloy)

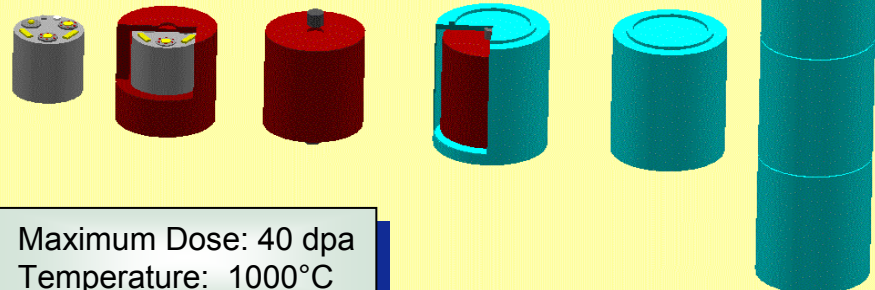
SiC<sub>f</sub>/SiC : 2D

SiC<sub>f</sub>/SiC : 3D

2 materials to be defined : TiN, SiC (other  
composition) NbZrC ?

**SAMPLES**

- Small Disk
- TEM Specimen
- Cylinder
- Small Beam



*Some specific University research areas of interest for the transmutation fuel development are*

- Fabrication process development for TRU bearing fuels
  - Process optimization & correlation of process parameters with irradiation performance parameters
  - Process modeling
  - Low temperature or low heat fabrication techniques for Am bearing fuels
- Fuel characterization techniques
- Design of separate effect irradiation experiments
  - Analyses of the irradiation experiments and resulting data
- Development of advanced PIE methods
- Development and assessment of advanced cladding concepts
- Development and assessment of advanced matrix materials for dispersion fuels/inert matrix fuels for LWRs and fast reactors
- Fuel concepts for advanced LWRs/High-burnup fuels
- Fuel concepts for GFR, design analyses and testing
- Design and assessment of remote fuel fabrication facility
- Advanced fuel modeling (atomistic scale to continuum scale to performance codes)



*Multi-institutional fuel development working group (FDWG) is well established and is essential in the successful conduct of the research activities*



Name	Institution	Primary Expertise
Todd Allen	UW	Clad materials
Richard Ambrosek	INEEL	Fuel irradiation
Doug Crawford	ANL	LFR system integration manager
Jess Gehin	ORNL	Mixed oxide fuels
Steve Hayes	ANL	Metal, dispersion and inert matrix fuels
Steve Long	LANL	Ceramic fuels
Stuart Maloy	LANL	Clad materials
Ken McClellan	LANL	Ceramic fuel characterization and modeling
Mitch Meyer	ANL	Metal, dispersion and inert matrix fuels
Kemal Pasamehmetoglu	LANL	National Technical Director, Chairman of FDWG
Eric Shaber	INEEL	Fabrication processes and TRISO fuel
Steve Sheetz	WSRC	Fuel deployment and facility design
Finis Southworth	INEEL	NGNP system integration manager
Mike Todosow	BNL	Fuel safety envelope
Jim Tulenko	UF	Fuel fabrication, modeling and IMF
Debbie Utterbeck	INEEL	Fuel irradiation
Kevan Weaver	INEEL	GFR system integration manager
Dave Williams	ORNL	TRISO fuel
Steve Willson	LANL	Ceramic fuels

*University research Pis will be invited to selected FDWG meetings:*

- to participate in the discussion; and*
- to present to status of their research*

